Lattice Vibrations of Tin Under Pressure

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Lattice vibrations provide an important contribution to equations of state (EOS) of materials important to the mission of Los Alamos National Laboratory. Lattice vibrations can in general be measured experimentally, but in practice this can be expensive or in some cases even dangerous.

Density Functional Theory (DFT) calculations of lattice vibrations present a path to improve EOS of materials under many conditions. A typical calculation costs significantly less than an experimental measurement, and materials that pose a risk in measurements can be treated on a computer just like harmless substances. Systematic calculations as a function of, for example, volume, become easily implemented.

In particular for systems at ambient pressure, experience shows that the DFT calculations of lattice vibrations agree well with experimental values. A collaboration with researchers of the High Pressure Science and Engineering Center (HiPSEC) at the University of Nevada, Las Vegas, indicates that this agreement holds for tin at higher pressures.

Figure 1 shows the lattice vibration dispersion calculated for tin in the body-centered cubic crystal structure with a volume corresponding to that found in experiments at a pressure of 64 GPa. The frequencies are plotted for sequences of wave vectors along high symmetry directions. Experiments can certainly measure such dispersions, i.e., the frequencies of particular wave vectors, but under pressure these measurements become much more difficult.

While still not a trivial task, the density of states (DOS) of the lattice vibrations of a crystal under pressure can be measured with less difficulty. Figure 2 shows the lattice vibrations DOS measured by HiPSEC researchers in excellent agreement with the calculated DOS. This agreement adds confidence to equations of state constructed using calculated lattice vibrations.

The collaboration with HiPSEC researchers continues with tin at other pressures where more complex crystal structures appear.

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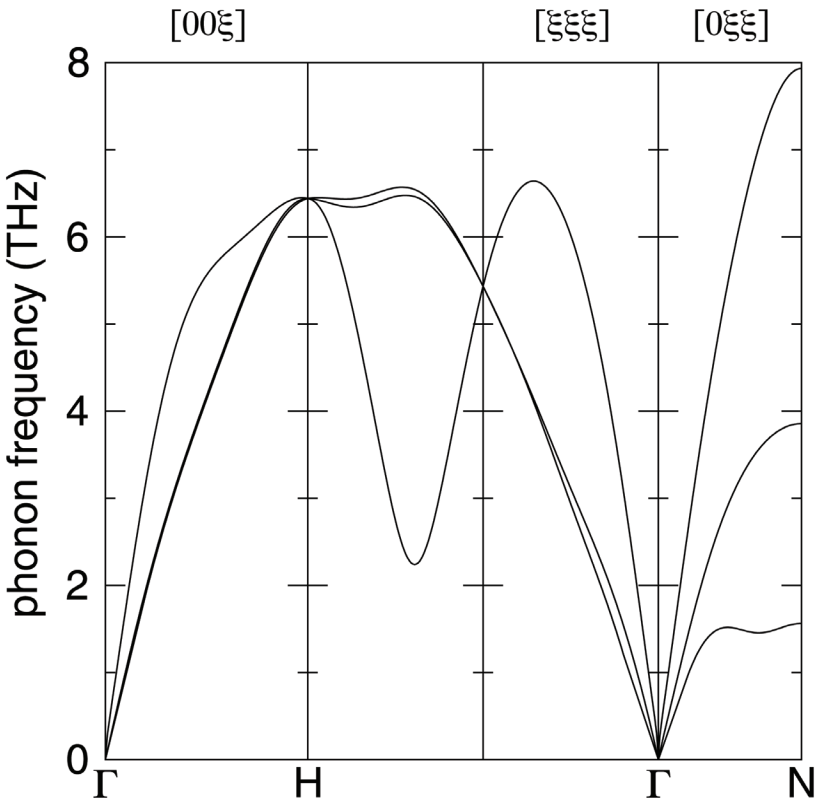

Fig. 1.
Calculated lattice vibration dispersion of tin in the bcc crystal structure with volume given by experiment at a pressure of 64 GPa.

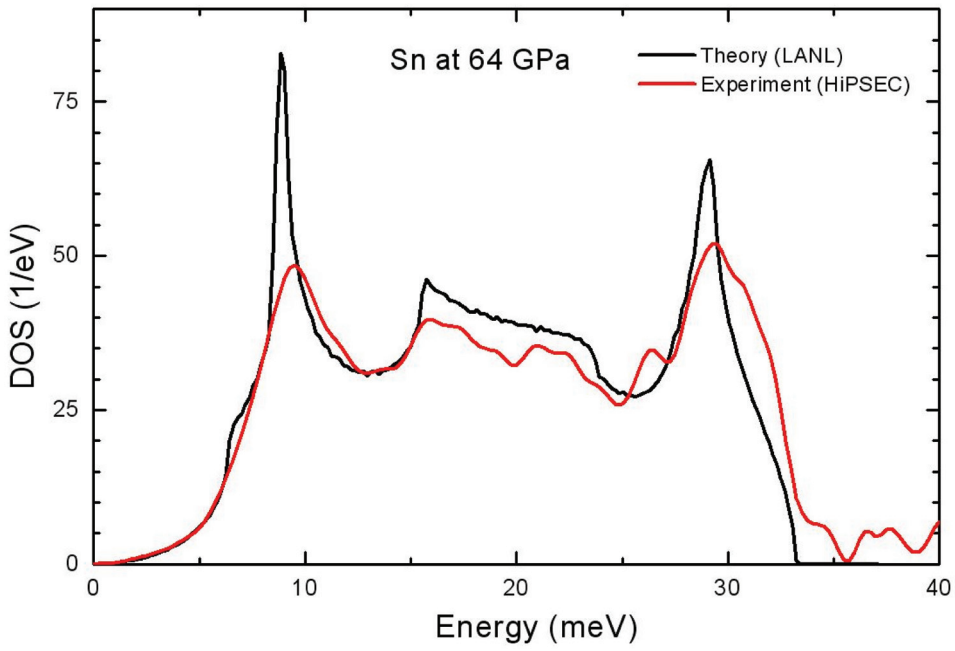

Fig. 2.
Lattice vibrations density of states (DOS) of tin at a pressure of 64 GPa.